

Formyl chloride
2565-30-2 | DTXSID30180344

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -52.9 °C

Global applicability domain: Inside

Local applicability domain index: 5.61e-01

Confidence level: 5.13e-01

Nearest Neighbors from the Training Set

Image not found

Chloroacetaldehyde

Measured: -16.3

Predicted: -51.1

Image not found

Acetyl chloride

Measured: -113

Predicted: -63.3

Image not found

Chloroacetyl chloride

Measured: -22.0

Predicted: -23.7

Image not found

Methyl chlorocarbonate

Measured: -61.0

Predicted: -57.5

Image not found

Acetic acid, 2,2-dichloro-, methyl ester

Measured: -51.9

Predicted: -49.3